HPC Simulations Save $4.3M in Development Costs

MSRC Director's Forum
Updates Add Power to ARL MSRC

Welcome to another issue of the Link. We have received feedback from you that you are pleased with the new version of our journal, and we're glad you like it! Our team has worked hard to develop a more useful and informative way for users to find out what's going on at the ARL MSRC, and we will continue to strive to serve you better.

This issue of the Link is packed with information on recent events, exciting projects, and the latest technology that we've added to serve the user community. It's been a busy few months, and I'd like to tell everyone about some of the exciting things we've been doing lately.

In November, the ARL MSRC hosted the HPCMP booth at Supercomputing 2002 (SC2002), one of our biggest conferences. This year, there were over 6,000 people in attendance at the conference, which was held in nearby Baltimore, MD. The ARL MSRC had the privilege of hosting the HPCMP booth this time around and enjoyed working with everyone to make it a success. As you can read in the pages of this issue, the hard work of the team paid off and the booth was a big hit with our users and the supercomputing community. I commend our staff and all contributors for the great job they did on the booth, including showcasing some of the exciting projects that are part of the HPCMP.

In December, our staff participated in the 23rd Army Science conference in sunny Orlando, FL. This year's theme, "Transformational Science & Technology for the Army...a race for speed and precision," highlighted the latest developments in emerging technologies and their impact on the soldier of the future. The conference site was transformed into a portable HPC scientific visualization center, which generated significant interest on the part of the attendees.

Also in December, the final touches were completed on the building modifications and associated infrastructure for the new scientific visualization collaboration center at ARL. As part of the new center, a new RAVE-II Immersive display system was installed by SGI and Fakespace. Phase two of the visualization center has begun and will integrate the existing ARL MSRC audio and video assets into a structure that will allow input sources to be displayed on the RAVE system.

Soon, the most powerful Linux-based system in the DoD HPCMP will be installed at the ARL MSRC as part of the Technology Insertion 2003. The 1.7 peak TeraFLOPS system will be built by Linux Networx and will have 256 3.06 Intel XEON CPUs available to ARL MSRC customers. In addition, the center will upgrade its unclassified IBM Power4 system, Shelton, to 128 1.7-GHz POWER4+ CPUs and a new interconnection network. We will also implement a significant enhancement of the mass storage archival system, increasing its tape and disk capacity and performance by more than a factor of two. The storage server platforms will be replaced with the latest technology to support the increased throughput capabilities of the new tape and disk devices. We look forward to providing these three significant additions to you.

Dr. Jim Newill and his team of researchers have been designing and developing more accurate munitions for the Abrams tank gun system. The ARL MSRC helped Dr. Newill and his team save $4.2 million in development and testing costs.

As you can tell, the entire ARL MSRC staff has been very active. We continue to focus our efforts on providing the best possible HPC environment to our customers, and we look forward to working with you as we continue our transformation into a communications-rich center. As always, we remain committed to fully supporting the DoD computational mission by providing complete solutions for all of your research challenges. In addition, we appreciate your comments, which can reach us via email at outreach@arl.army.mil.

We will meet again soon.

Charles J. Nietubicz

Mr. Charles J. Nietubicz is the Division Chief of the High Performance Computing Division (HPCD) and Director of the Major Shared Resource Center (MSRC), Computational and Information Sciences Directorate (CISD), Army Research Laboratory (ARL).

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Cover Artwork By Robin Gravels

ARL MSRC Hosts IBM Power4 System Seminar

On 19 December 2002, Mr. Jim Tuccillo from IBM Federal came to the ARL MSRC to present information relating to the new IBM Power4 systems that were recently released into the production environment. During the course of the class, all aspects of the Power4 were discussed from an overview of all the hardware related to the system, to performance issues dealing with both hardware and software, to code development concerns. Several issues appealed directly to the user community in attendance, including compiler flags, MPI communication information, and performance issues between the MSRC's existing Power3 system and the new Power4 system. In addition to Mr. Tuccillo's presentation, Mr. Steve Thompson from Raytheon at the ARL MSRC presented information and answered questions relating to the GRD batch queuing system.

ARL MSRC Attends IBM Supercomputing Users Conference

The IBM SP XXL Group Winter meeting was held at the Maui High Performance Computing Center during the last week in January 2003. The XXL user group is comprised of computing sites that meet the minimum IBM compute system requirements and contribute to the advancement of high performance computing on IBM systems. The ARL MSRC was voted into the group in the summer of 2001 after installing a 512-processor IBM Nighthawk 2 system and has been represented at every meeting since becoming a member. IBM views the group as a strong voice and advocate and takes heed of any and all suggestions, complaints, and concerns the group expresses.

The week-long 2003 winter meeting, attended by ARL MSRC's Mike McCraney, produced an annual report not unlike others produced in past years. Issues ranging from the handling of problem reports by the customer services staff, to design deficiencies, to systems administration hurdles caused by poorly planned upgrade paths were identified. The summer meeting will be held in late July at the Center for Scientific Computing in Helsinki, Finland, where the group will review IBM's response to each item in the annual report.

Technology Insertion 2003

As part of Technology Insertion 2003 (TI-03), a proposal for HPC expansion was developed by all four MSRCs in cooperation with the HPC Modernization Office to meet user needs and type of processing that each center expects for support in the next year.

Under the upcoming TI-03 upgrades, the ARL MSRC plans to boost the size and strength of the unclassified IBM p690 system, Shelton. Sixty-four additional 1.7-GHz Power4 processors will be integrated into the system, and the existing 64 processors will be upgraded from 1.3 GHz to 1.7 GHz clock speed. The system will maintain a balance of 1 GB of RAM per processor with the addition of 64 GB. Interconnect support will also be upgraded from the existing Colony/Corsair adapters to the new Federation switch. These upgrades will more than double the current compute power of the existing system – from 333 to 870 GFLOPS. Once installed, the new/upgraded system will be configured as four 32-processor nodes connected with the Federation switch. These upgrades are expected to be installed and integrated late this summer or early fall.

Another part of TI-03 upgrade includes the implementation of a significant enhancement of the mass storage archival system, increasing its tape and disk capacity and performance by more than a factor of two. The storage server platforms will be replaced with the latest technology to support the increased throughput capabilities of the new tape and disk devices.

Also exciting is the fact that the ARL MSRC, the DoD High Performance Computing Modernization Office, and Linux Networx have reached an agreement that will lead to the installation of the most powerful Linux-based system in the DoD High Performance Computing Modernization Program. The new cluster will have 256 3.06-GHz Intel XEON CPUs available to users and an additional 27 2.4-GHz CPUs for system management and parallel file system support. The system will also support a peak performance of 1.7 TeraFLOPS, making it the second most powerful machine at the ARL MSRC.

APG Collaboratorium Opens

In December 2002, the new Aberdeen Visualization Center opened. This state-of-the-art facility has exciting new technical capabilities, including the RAVE-II Immersive display system. The center provides the ARL MSRC scientific visualization team with fully integrated, 3-dimensional study and analysis tools for use in various research and development projects. Starting in March, Fakespace and SGI will integrate the existing ARL MSRC audio and video assets into a structure that will allow these input sources to be displayed on the RAVE.

ARL Visits NASA, Attends Nanotechnology Alliance

During March, ARL staff visited NASA's Goddard Space Flight Center to discuss drafting specific plans for technical and scientific collaborations with NASA concerning the application of ARL and NASA expertise in nanotechnology to space systems. The Army's plans to examine an additional dimension of space through a synergistic relationship with NASA is made possible through NASA's existing fabrication and manufacturing infrastructure suited for space systems. Also in March, ARL representatives attended the first meeting of the Greater D.C. Nanotechnology Alliance at the Applied Physics Laboratory of Johns Hopkins University.

Dr. Whalin receives the Meritorious Civillian Service Award from General Kern during his retirement ceremony.

Whalin Retirement

In February, Dr. Robert W. Whalin retired as Director of the Army Research Laboratory, a position he has held since 1998. Dr. Whalin is going back to his home state of Mississippi, where he will be the Associate Dean of Engineering at Jackson State University. While Dr. Whalin will be greatly missed, we wish him all the best on his retirement and new endeavors.

Mr. John Miller and Ms. Jill Smith

Miller and Smith Named Acting ARL Directors

Mr. John Miller is currently serving as the Acting Director for the U.S. Army Research Laboratory. In his previous position as the Associate Director for Plans, Programs, and Budget, he was responsible for strategic and operational planning, resource allocations, and program formulation and direction.

During his civil service career, Mr. Miller has served in a number of positions in ARL and prior to that in the U.S. Army Harry Diamond Laboratories. From 1992 through 1998, he held positions as Division Chief, Acting Director of the ARL Sensors Directorate, and Deputy Director of the ARL Sensors and Electron Devices Directorate.

Mr. Miller holds a bachelor's degree in Aerospace Engineering and a master's degree in Mechanical Engineering, both from the University of Maryland, and is a past recipient of the U.S. Army Research and Development Award.

Ms. Jill Smith is currently serving as the Acting Deputy Director for the U.S. Army Research Laboratory. Previously, she served as the Director of the Weapons and Materials Research Directorate.

Ms. Smith has worked extensively in the areas of high performance computing and networking, creating the Army's first supercomputing network and leading many efforts in these areas for U.S. Air Force Air Mobility Command, Department of the Army, and Department of Defense, including consultation to the White House Office of Science and Technology Policy. In addition, she has many publications in the ballistics research area including survivability, lethality, model validation, live-fire testing, and many other topics.

Ms. Smith received both her bachelor's degree and master's degree in Mathematics from Shippensburg State College in Pennsylvania. She completed additional graduate work in Statistics and Electrical Engineering at the University of Delaware.

Dr. Raju Namburu and Dr. Andrew Mark with Ms. Jill Smith, Acting Deputy Director, ARL, who presented the awards

ARL Scientists Receive Awards

Drs. Andrew Mark and Raju Namburu recently received commendations for exceptional service as Computational Technology Area (CTA) Leaders from the Office of the Director of Defense Research and Engineering for their support of the DoD High Performance Computing Modernization Program (HPCMP) at the ARL MSRC.

Dr. Andrew Mark, Chief of ARL's Computational Sciences and Engineering Branch was commended for his work as the Integrated Modeling and Test Environments (IMT) CTA Leader. While IMT CTA Leader, Dr. Mark served as the HPCMP's key scientist, bringing high performance computing to the test and evaluation community and providing key technical and management advice.

Dr. Namburu was commended for his service as the ARL MSRC CTA Leader for Computational Structural Mechanics, and was praised for providing key technical and management advice to the users of his scientific community as well as managing Weapon-Target Interaction (WTI) programs and collaborating with his fellow researchers for the WTI program's contributions to mission success.

The Little NGEN That Could
By Michelle Morgan-Brown with Mark A. Bolstad and Dr. Michael J. Nusca

At the ARL's Weapons and Materials Research Directorate, Aerospace Engineer Dr. Michael Nusca and his Propulsion Physics team are working with the ARL MSRC's Scientific Visualization Team and Mark Bolstad to solve a very complex, coupled set of partial differential equations that simulate the real-time ignition, combustion, and flame spreading of modular gun charges for indirect fire weapons. Over the last couple of years, the Department of Defense has recognized this as what is known as a high performance computing "Challenge" project because it "requires vast amounts of computer memory, significant computer speed, and real-time scientific visualization of very large datasets in order to produce an accurate simulation of the propelling charges and so a clear understanding of the fundamental physics behind them," says Dr. Nusca.
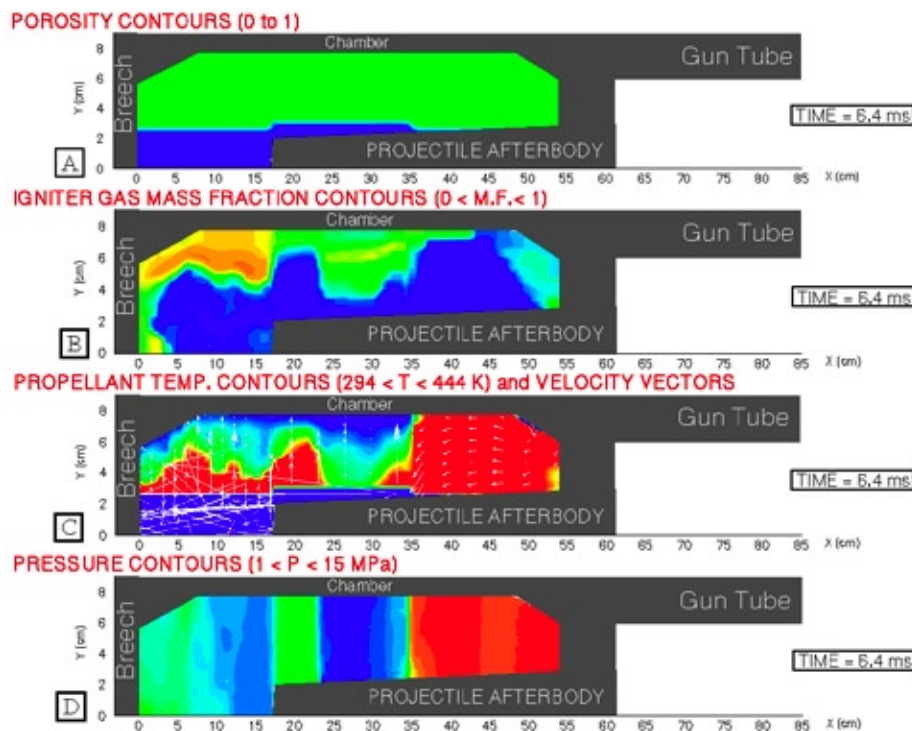

Figure 1. For a HLD gun charge made up of SP in disk and granular forms and for a short time after functioning of the igniter system, these figures show the computed (A) porosity contours, (B) igniter gas mass fraction contours, (C) temperature contours for propellant along with velocity vectors, and (D) gas pressure contours.

In order to run these simulations, Dr. Nusca and his team use a complex computer program called the Next Generation Interior Ballistics code, or NGEN, which was developed here at ARL. NGEN is a computational fluid dynamics (CFD) code that, in this case, solves the 3-dimensional conservation equations for both the gas and solid phases. In other words, the code allows a multiphase simulation, which Nusca says is "essential for the simulations of these [modular] charges."

The NGEN code has been under development by the Army for the past nine or ten years. However, for the first eight years of that, engineers like Nusca and his team did not have the scientific visualization available to them that would allow them to visualize both the gas phase

and the burning propellant particles. The tools and the visualization knowledge that Dr. Nusca needed were unavailable to him; therefore, he turned to the ARL MSRC and Computer Scientist Mark Bolstad for help.

Bolstad took the data from Nusca's code and wrote custom converters to put the code output into the format used by EnSight, one of the main tools for visualization at the ARL MSRC. As he was visualizing the results and looking at the various combinations of variables that Nusca wanted to see, Bolstad notes that he "happened to notice that there was something amiss in the data."

What Bolstad saw in the visualization was that after a rupture (i.e., break or burn through) in one of the propellant container walls occurred, this breach re-sealed itself, which, they both agreed is physically impossible. When he saw these results, Bolstad called Nusca and let him know that something looked wrong. During the call, Nusca was able to view the visualization from his office workstation, while Bolstad pointed out the features that he thought were inconsistent with what should be happening in this visualization.

Given the time step and grid cell where the inconsistency occurred, Nusca was able to trace through the code and discover an error in a little-used portion of the code: the section used for restarting the simulation from a given time step. While this error only affected the input/output on a code restart, the subtle consequences in the simulation were significant. That is, the timing sequence of propellant ignition in the modular charges had changed.

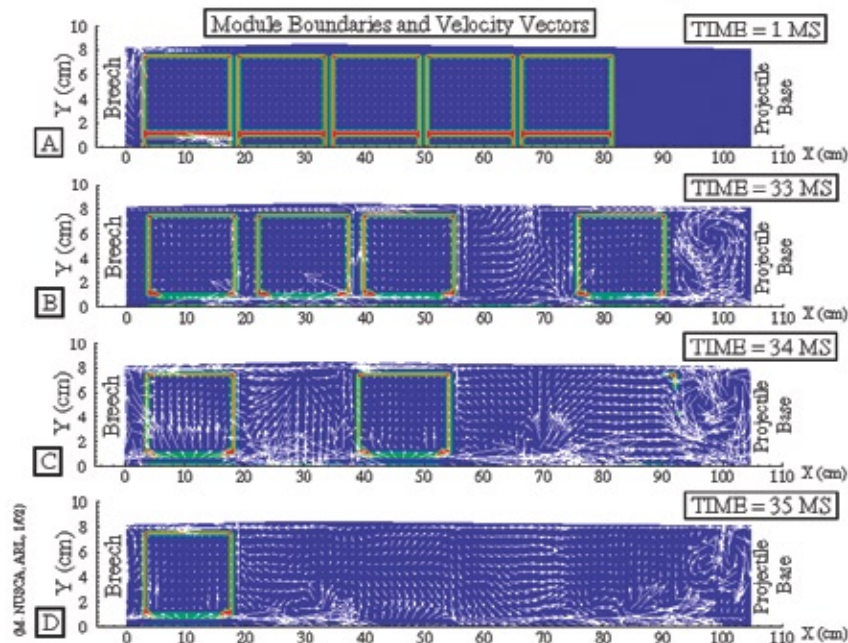## ARL-NGEN3 CODE SIMULATION OF M232 MACS CHARGE (ZONE 5) IN XM297 CANNON

Figure 2. For a the MACS gun charge made up of SP in five separate modules and for 1 to 35ms after functioning of the igniter system, these figures show the computed module boundaries (location and integrity) along with gas flow velocity vectors.

multiphase CFD code capable of producing detailed simulations of a very complex gun propellant charge system. The Army's legacy force weapons require this charge system; therefore, such simulations, which help optimize the charges, are absolutely essential to the Army's mission. However, human eyes can only see so much within the vast array of numbers produced by these simulations. The "eyes" of the ARL MSRC's computer scientists are their scientific visualization tools. These eyes, when trained on the simulations of these gun charges, saw some imperfections. Upon correction, the "little NGEN that could" happily chugged along, utilizing high performance computing assets and producing simulations that are much more meaningful (and colorful) than black smoke.

For size comparison, this data inconsistency occurred in only 0.00006% of the entire dataset. Without visualization, this error would probably have never been found. Owing to precision pinpointing to where the error had occurred within the dataset, scientific visualization also reduced the time necessary to fix this coding error.

The gun charges being studied are part of the Army's modular charge system in which the soldier loads the number of charges into the weapon that are appropriate for the range to the target. Dr. Nusca, leader of this computing Challenge project, notes that "the simulation of these [charges] inside the gun's combustion chamber is quite complicated, but is essential to the Army's charge development and its understanding of the physics behind these charges."

In the end, this is the story of ARL engineers, computer scientists, and high performance computers. The engineers developed a

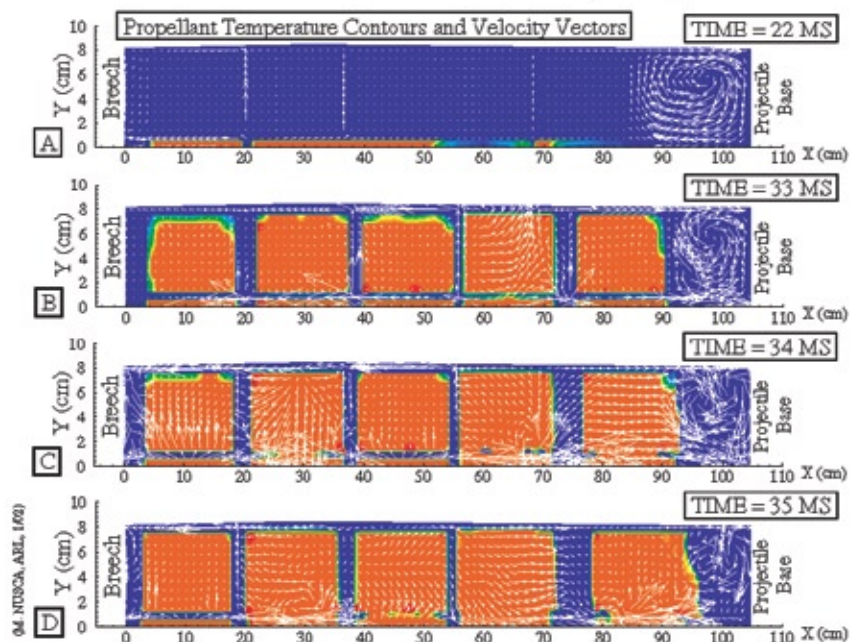## ARL-NGEN3 CODE SIMULATION OF M232 MACS CHARGE (ZONE 5) IN XM297 CANNON

Figure 3. For a the MACS gun charge made up of SP in five separate modules and for 22 to 35ms after functioning of the igniter system, these figures show the computed propellant temperature and gas flow velocity vectors.

What's All This Reality Sandwich Stuff, Anyhow?

By Jerry Clarke and John Vines

On the red-eye flight from Los Angeles to Baltimore, an overworked, underpaid U.S. Army Computer Scientist gazed pensively out of the air ship's porthole. As the weary mass of travelers passed thirty thousand feet over another of the countless cities illuminated by the twinkle of street lights and strip malls, he wondered which personality flaw had caused him to promise his innovative but demanding director capabilities which he was not even sure were possible … again! Just then, he saw an object appear to hover just above the jet's wing about 10 feet from his window. The object was a semi-transparent, box like structure that floated outside, clearly defying established laws of Newtonian motion. Mental images of a similar "Twilight Zone" episode with a young William Shatner convinced him that an attempt to verify the existence of this object by awakening the slumbering passenger to his left might not be the most prudent course of action.

Digital Flat at ICT's FlatWorld.

Digital Flat with projected synthetic environment.

So there he sat, doubting his own senses, not to mention his sanity, staring at something that could not exist. Upon closer observation, he noticed a human hand was attached to the object. He also became aware of a rustling sound across the aisle that was synchronized with the object's motion. Aha! Just like the Haunted Mansion at Walt Disney World, the object that had captivated his interest was, in reality, just a reflection of a passenger across the aisle reaching into the overhead bin to retrieve her carry-on bag. The effect is known as "Pepper's Ghost," named for Professor John Henry Pepper who first developed the technique in the latter part of the 19th century. What our sleep-deprived traveler had haplessly stumbled upon, besides a cheap parlor trick, was a way to fulfill the ludicrous promises he had made just a few hours ago!

The previous afternoon, he had been at the Institute for Creative Technology and seen a demonstration of FlatWorld by its Project Manager, Jarrell Pair. FlatWorld uses Hollywood set construction techniques along with large rear projection screens, to provide a cost effective, scalable, configurable training and simulation environment. Real objects, like door frames and free standing window frames, are placed in front of rear projection screens that are driven by projectors to give the illusion of brick or plaster walls. When the user opens the door or window, the computer simulation causes virtual helicopters or adversaries to appear in the opening. This "mixed reality" environment is augmented with 3D sound and makes for quite an impressive demonstration.

"Can we use this technology for physics-based simulations?" the Director asked. "Sure we can!" blurted the Computer Scientist, without realizing the ramifications of those three words, as usual! Without hesitating to continue digging the hole in which he had stepped, he added, "We could add to this and make something available nowhere else." His fate was sealed; exactly how does one use mixed reality for scientific visualization? How does one add real objects to virtual space without seeming contrived? Windows and doors are hardly applicable to scientific data. Besides, as soon as one puts real objects in front of a stereoscopic projection, the light is blocked, defeating the 3D illusion.

Professor John Henry Pepper, it would seem, provided the answer over a century ago. By placing the virtual objects "in front of" real objects (not possible with traditional screen projection), an Augmented Virtuality experience is made possible. By adding a traditional rear projection screen behind the real object, one creates a "Reality Sandwich" where virtual objects can be both in front and behind real objects and people.

ARL has developed a prototype of this Augmented Virtuality Scientific Data Center by using commodity components (2.8-GHz PCs, InFocus projectors, consumer 6.1 audio system, etc.) and a local hardware store (bathroom mirrors, 2x4 lumber, channel strut steel, etc.).
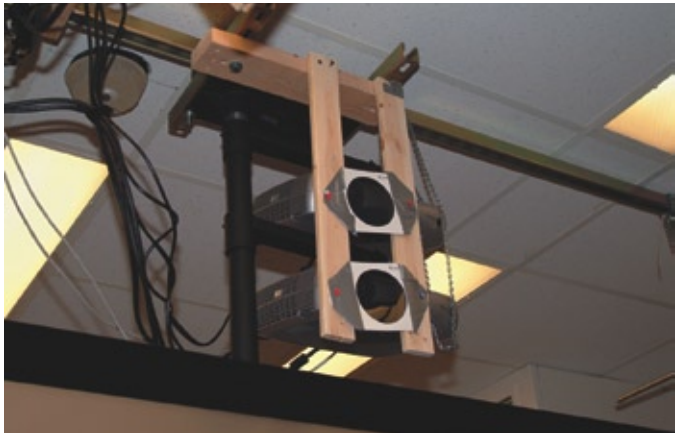
Prototype rear projection passive stereo configuration.

A transparent screen material is rear projected from above. Real objects are placed behind the transparent screen. A standard rear projection screen is placed behind the real objects. Currently the system is used to explore volumetric results from a Computational Electromagnetics simulation. With a real object or presenter in between the two screens, the data appears to be suspended in space. The addition of positional 3D audio allows a probe to be inserted into the data, which changes pitch in relation to the calculated data. The direction of the sound changes to correspond to the position of the probe.

Prototype "Reality Sandwich" configuration.

We're currently developing software based on existing de facto standards to allow data from many different computational technology areas to be experienced with the system. By utilizing distributed visualization techniques, we add multiple screens, each driven by a separate PC, resulting in a scalable environment … all as a result of a choosing a window seat.

Light Stage Captures Imagination at Army Science Conference
by Michelle Morgan-Brown

The Light Stage 3 was developed by Dr. Paul Debevec, Executive Producer of Graphics Research, and his team at the University of Southern California's Institute for Creative Technologies. This new technology focuses 156 red-green-blue light-emitting diode (LED) lights toward an actor, who is filmed simultaneously with a color camera and an infrared matting system. The actor is superimposed on a background and appears to be in a created or previous filmed background. Sure, we've all seen this before in movies like "Star Wars" and "The Lord of the Rings," but the Light Stage 3 isn't using blue screen technology. Rather, it recreates the exact lighting of the environment the actor is immersed in, down to shadows, highlights, shading, and indirect illuminations or reflections. The end result is a much more realistic image than most of us are used to seeing at the movies.

The Institute for Creative Technologies (ICT) was created in 1999 by the U.S. Army to enlist the resources and talents of the entertainment and game development industries and to work collaboratively with computer scientists to advance the state of immersive training simulation. The goal of the ICT is the creation of the Experience Learning System (ELS), which provides the ability to learn through active, as opposed to passive, systems.

This exciting new technology was shown at the 23rd Army Science Conference in Orlando, FL, during the week of 2-5 December 2002. The Army's interest in this technology is for training purposes, as the warfighter can train using such simulations that are closer to real battlefield environments. The Army cannot only put a person in an immersive environment, but it can also put vehicles or other equipment in the same immersive environment and run training simulations that are, again, more realistic than the current training simulations used. Since Light Stage 3 requires a large amount of computing power, HPC systems are essential to its almost real-time images.

This technology, while exciting for many training and educational possibilities, is so new that all of the uses for it are not yet obvious. Time and research will show what Light Stage 3 can do. You never know. It may soon be at your local movie theater, in your computer games, or even at your office – you just won't know you're seeing it.

Computational Chemistry:

Anti-Malaria Drug Research

By Dr. Mark Zottola

Dr. Mark Zottola of High Performance Technologies, Inc. (HPTi) is the Computational Chemistry on-site lead for the Programming Environment and Training (PET) team at the U.S. Army Research Laboratory (ARL) and has been collaborating with Dr. Jean Karle, a recognized world leader in anti-malarial research. Dr. Karle is also a member of the research team at Walter Reed Army Institute of Research (WRAIR). The PET team seeks to help introduce DoD researchers to the power of high performance computing. Once researchers realize the scope of problems that can be handled by high performance computing, their productivity can exponentially increase. The ability to handle large computational systems and ask questions which cannot be answered via experimental techniques are two of the greatest assets of high performance computing.

Drs. Zottola and Karle's work involved classical drug design techniques utilizing high-level quantum mechanics calculations on derivatives of Qinghaosu, a traditional Chinese medication for malaria. Qinghaosu and its derivatives are rather large molecules comprised of over 40 atoms each. In order to accurately model these molecules, calculations required over 43,000,000 integral evaluations. The scope of this problem was unworkable just a few

Representation of Qinghaosu (rendered in blue) in the binding pocket of Falcipain-2. The structure of Falcipain-2 is rendered in cartoon format to more clearly show the structural elements of the protein.

years ago. Further, this problem dictated an amount of memory, disk space, and computational speed only available on a supercomputer (such as those available at the ARL MSRC). Drs. Zottola and Karle's work required several thousand CPU hours on both the IBM Power3 and SGI Origin 3800 machines. These jobs routinely required the simultaneous use of 8 to 16 processors.

Much work has been done at WRAIR on developing effective anti-malarial treatments. Malaria, spread by the anopheles mosquito, infects half a billion people yearly, killing nearly 1.5 million children a year. This is a global medical issue. Malaria has been virtually eliminated in most developed countries due to effective anti-mosquito and land management programs However, malaria still poses a threat to people living in tropical and subtropical climates. In combat theaters, malaria is the primary factor degrading combat efficiency. Further, the incidence of malaria increases in regions where there is poverty and hunger. Poverty and hunger contribute to political instabilities affecting our allies in these regions of the world. As a result, the Army and the World health Organization (WHO) have teamed together to fight this global scourge.

Researchers around the world have been modifying Qinghaosu. These modifications were done in order to obtain more potent treatments for malaria. Much effort has been expended in this area due to the considerable challenges in developing anti-malarial agents. The first challenge is the fact that the agent must be active against a broad spectrum of malarial parasites. In the field, it is difficult to diagnose which parasite has infected the person. The second problem lies in treating those who succumb to severe malaria. Often, drugs must be delivered intraveneously (IV) to unconscious patients. Hence, the drugs used to combat the parasite need to have substantial water solubility. Currently most drugs are derivatives of Qinghaosu, and these have poor solubility characteristics in water. Finally, the anti-malarial agents studied at WRAIR have a significant side effect. Prolonged use or high dosages results in an ototoxic response leading to the destruction of hearing centers. At still higher doses, Qinghaosu induces shutdown of the autonomic system. Since this ototoxicity is due to transport across the blood-brain barrier, design for newer anti-malarial agents needs to focus on decreasing the ability of Qinghaosu derivatives to be transported across this membrane.

In order to meet these challenges, the mechanism of action for Qinghaosu must be understood. Yet, until recently, little work had been done to understand exactly how these molecules worked. This understanding is crucial since it would streamline the design process leading to more powerful and easier to synthesize anti-malarial treatments. This streamlined process would then reduce the time required to bring an effective treatment to both the Army and the WHO. The distribution of this medicine by the WHO would diminish the devastating effects of this disease. By removing this disease, the cycle of poverty in third-world nations can be broken, leading to enhanced world stability.

Dr. Mark Zottola gives an informal presentation at the 23rd Army Science Conference. (See page 20 for conference details).

Using the resources available at the ARL MSRC, Drs. Zottola and Karle were able to develop and computationally validate a mechanism of action for derivatives of Qinghaosu. This mechanism led to a model to predict the ability of Qinghaosu derivatives to treat malaria. A screen for toxicity to the malarial parasite was developed at WRAIR. The computational model derived from calculations at the ARL MSRC showed a 92% correlation between the predicted and actual values of parasite toxicity for a series of Qinghaosu derivatives. This high level of correlation against a live screen was strong validation of the proposed mechanism of action. With this validated mechanism, researchers at WRAIR now have a tool to more efficiently design Qinghaosu derivatives with enhanced anti-malarial activity, improved water solubility characteristics, and a broad-band spectrum of activity against all types of malaria-causing parasites and a design tool to avoid the problems of ototoxicity.
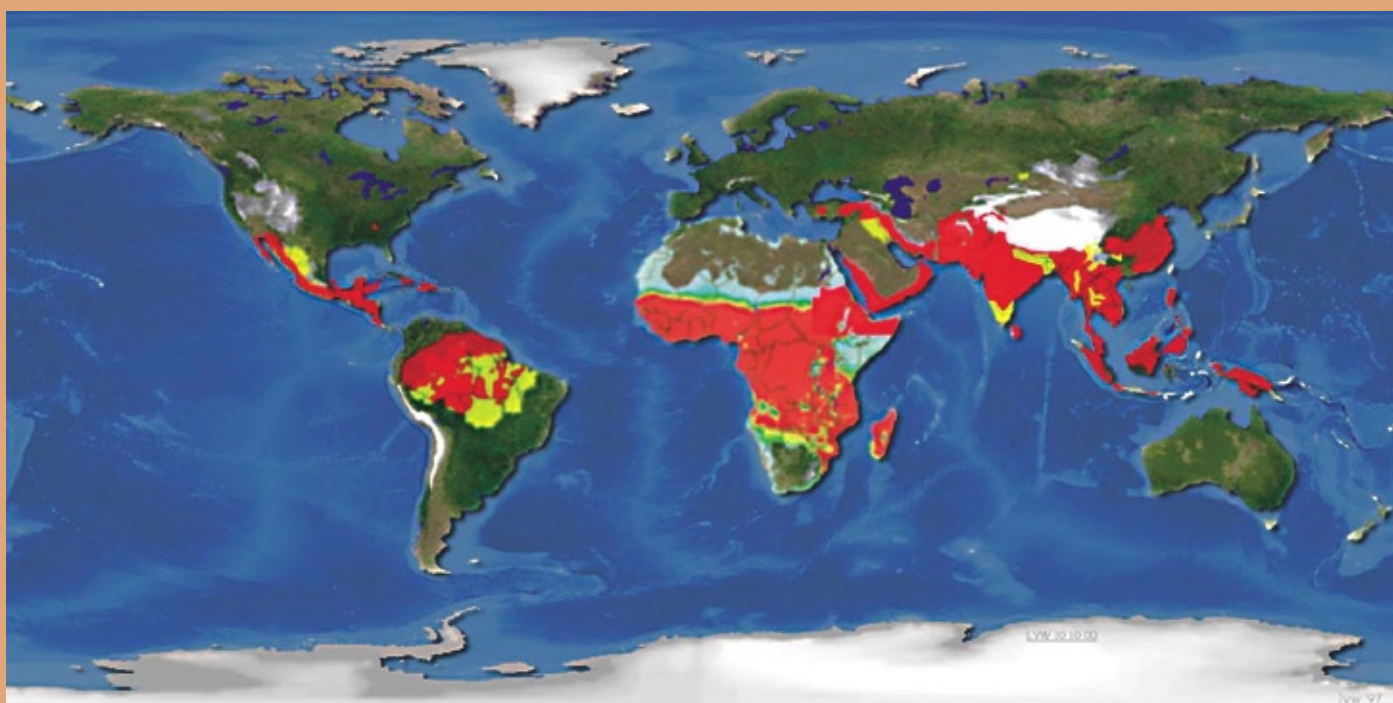
World map of malaria-prone areas (shown in red).

Insights from the Terabyte Crowd:
Supercomputing 2002

By Michelle Morgan-Brown

From 16-22 November 2002, the ARL MSRC team attended Supercomputing 2002 (SC2002) in Baltimore, MD. Every year, this conference brings together the world's supercomputing community to discuss the future of high performance computing, networking, and data technologies. This year's theme, "From Terabytes to Insights," was used in the High Performance Computing Modernization Program (HPCMP) booth to illustrate how the DoD uses high performance computing technologies to deliver scientifically based solutions to the warfighter.

Besides the many interactive presentations, lively talks, and demonstrations available on the floor of the conference, the technical program featured an exceptional set of speakers who addressed significant technical and real-world HPC application issues. In addition, the tutorials and education

The Land Warrior demonstrates the capabilities of the remote sighting system.

The HPCMO display booth at SC2002. The round device in the foreground is the Elumens VisionDome.

program provided unique opportunities for learning, and panel discussions were held for interaction and discussion by the supercomputing community.

This year, the ARL MSRC sponsored the HPCMP booth, which showcased new technology for the warfighter, including interactive demonstrations, technical presentations, and static displays. Preparation began early in 2002 for the conference since we had to coordinate the efforts of many

geographically dispersed groups, including the Modernization Office, four Major Shared Resource Centers, and numerous Distributed Centers. Our conference team worked very hard, and thanks to them our booth was highly praised as well as a big success. (See related story on page 26.)

Among the DoD's high performance computing technologies on display at the HPCMP booth were several Plasma screens highlighting the DoD's HPC successes, a portable Fakespace ImmersaDesk, and an Elumens VisionDome. In addition to the booth demonstrations and interactive presentations, the ARL MSRC also brought two static displays to the conference this year: the Land Warrior system and an Army vehicle known as an FMTV.

One of the crowd pleasers at SC2002 was the Land Warrior. This state-of-the-art system was designed for the warfighter and is part of the Army's Future Combat System (FCS). The research performed at the ARL MSRC makes such systems possible by significantly reducing development time and cost. The unique Land Warrior system integrates high-tech equipment with small arms, enabling the soldier to fight and win on the 21st century battlefield. Furthermore, it is designed to provide a greater degree of lethality, survivability, and command and control to the warfighter. The subsystems of Land Warrior include weapons, integrated helmet assembly, protective clothing, computer/radio, and software. The weapon system includes a video camera and an infrared sight, which will allow the ground soldier to operate in

any type of weather as well as at night. In addition, the helmet assembly has a night sensor, a laser detection module, a microphone, and a headset, while the protective clothing includes modular body armor and chemical/biological protective garments. The soldiers who will actually be using this system have been consulted on every step of its evolution, so the Army is sure that the system will perform for its soldiers in the real world.

FMTV truck during testing at Aberdeen Test Center.

Another impressive display was the Army's Family of Medium Tactical Vehicles (FMTV). The Aberdeen Test Center (ATC) was unable to house the amount of data generated by the many FMTVs they were testing, so they turned to the MSRC to provide them with the use of the latest advanced computing, data storage, and networking technologies to meet their needs. Using HPC resources allowed researchers to pinpoint design flaws in vehicles while they were being tested, and these resources also enhanced vehicle performance while minimizing cost and complexity and delivering significant weight reduction. HPC technology also allowed engineers to explore more design options. All of this, in turn, allows the Army to save money and valuable time during the design process.

Participating in SC2002 is always a rewarding and challenging experience for the ARL MSRC team, and we had a great time, as always, this year. Perhaps you came to the conference and visited our booth. If so, we hope you learned something more about the DoD's high performance computing efforts, saw something interesting, or at least enjoyed yourself. We hope you were as excited as we were to see our fellow supercomputing folk as well as the cutting-edge technology that will be coming our way soon. See you next year!

TeraBurst Gives SC2002 Demos a Boost

By Michelle Morgan-Brown and Dr. Robert Cromp

Supercomputing 2002 (SC2002) is a showcase for new technology, so naturally the ARL MSRC brought some of its cutting-edge scientific visualizations to show off at the HPCMP booth. Some of the most exciting demonstrations were of real-time, remote scientific visualizations of complex data sets, which required a tremendous amount of computing power. Due to the complexity of these data sets, the ARL MSRC used an SGI Onyx 3600 to power the visualizations. Naturally, it was logistically impractical to bring such a large computer to the floor of SC2002 in Baltimore. That's where TeraBurst Networks stepped in to help. Instead of bringing the Onyx 3600 and its data to Baltimore from ARL, TeraBurst brought the data to us.

TeraBurst did this by way of their Visualization To Optical (V2O) system, which allowed remote, real-time projection of high-resolution, 3-dimensional graphics from ARL's Adelphi, MD, site to the HPCMP booth 22 miles away.

The ARL MSRC was able to demonstrate visualization programs, including the Weather Model, ZSU anti-aircraft vehicle, and Ladar, utilizing the TeraBurst Networks system. In addition, we were able to remotely manipulate the data in Adelphi while on the floor of SC2002.

Currently, the ARL MSRC is pioneering a new technological breakthrough allowing real-time collaboration between high-resolution, 3D visualization centers. This capability may prove to be a valuable tool for researchers in many different disciplines and industries.

TeraBurst Networks develops high-performance, intelligent optical networking systems and collaborative visualization solutions to enable real time interactive collaboration of high-bandwidth video applications over wide area networks.

SC2002 Booth a Success
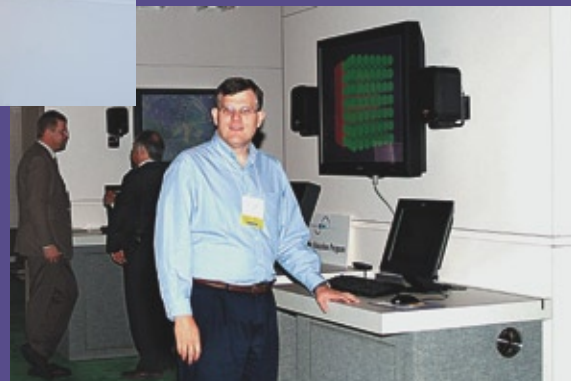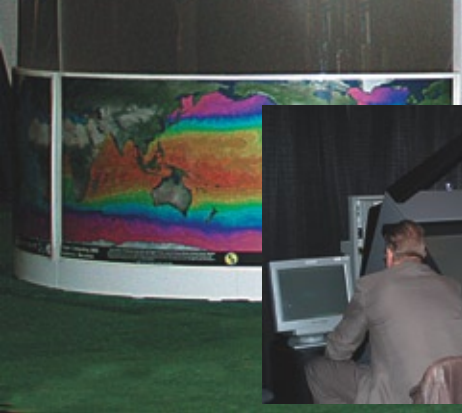
One Shot, One Kill
By Michelle Morgan-Brown

When Dr. James Newill wanted to gain a better understanding of the Abrams tank gun system to improve projectile launch accuracy, he turned to the ARL MSRC to help.   Dr. Newill is the Leader for the Computational Structural Dynamics Team, Aerodynamics Branch, Ballistics Weapon Concept Division (BWCD), Weapons Material Research Directorate at ARL, where he is primarily responsible for in-bore launch accuracy and understanding how projectiles interact with gun systems.

Typically, he works with the M1/A1, M1A2, and M1A2 SEP Abrams tank systems, which use the 120-mm, smooth bore M256 cannon. This is a precision, direct fire weapon where accuracy is of the utmost importance. The goal is one shot, one kill, where a target is on the order of a meter by a meter and is often several miles away.

Currently, the state of the art in precision jump experiments (the experiments that compliment this work) does not provide any information on the projectiles behavior in-bore, but only provide an indirect look at projectile's behavior in-bore by defining the state (transverse cg velocity and angular rates) of the projectile as it exits from the gun. High performance computing and scientific visualization at the ARL's MSRC allows Dr. Newill and his team to gain direct insight into the behavior of the projectile during the application of 1.25 million pounds of force (resulting in 75,000g of acceleration) over the 6 ms it takes to travel down the gun. Primarily, this research is used to understand how the structure of the projectile affects launch accuracy.
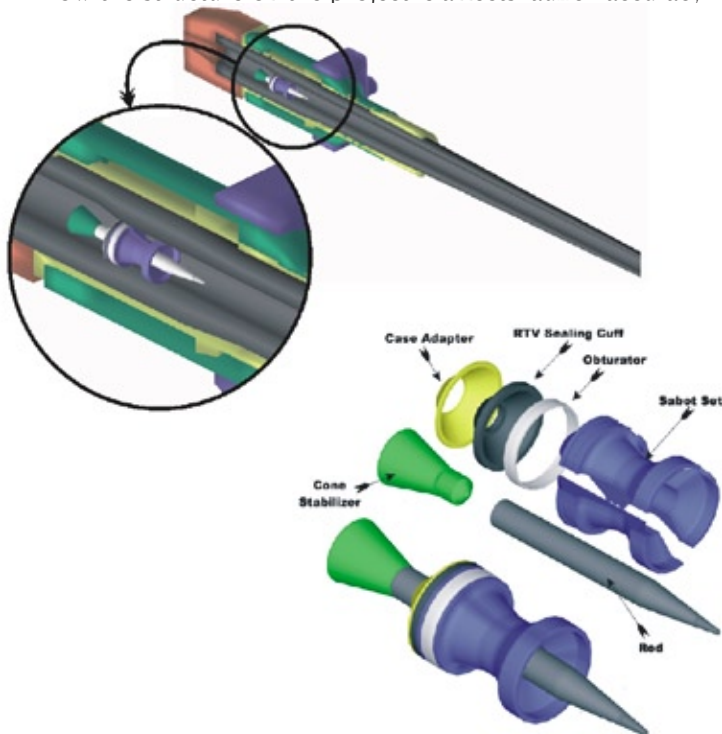
Computational models of M256 cannon with recoil, M865 KE Trainer.

This research allows the projectile teams to understand early in the development process how a projectile interacts and is influenced by the gun system during launch. This understanding allows accuracy to be built into the projectile as one of the considerations of design. This approach also provides methods for assessing the performance of improvements or modifications before expensive hardware is manufactured and tested.
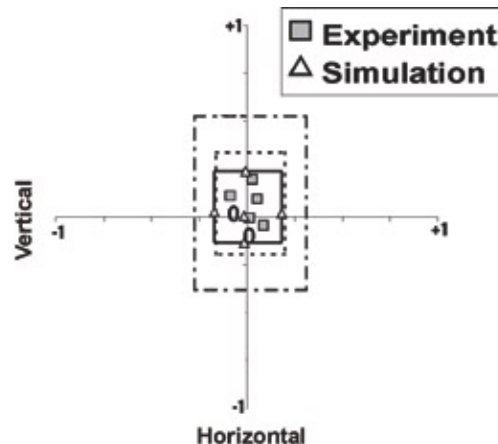

Angular rate comparison at the muzzle using simulation and experiment (jump test) data.

This research produces more accurate projectiles, and more accurate projectiles not only increase lethality (if you can't hit a target, the effectiveness of the lethal mechanism doesn't matter), but also translate into better survivability for tank personnel and vehicles. Accuracy is related to survivability for a tank since better accuracy allows crews to engage at longer ranges and win battles before the enemy can effectively fight back. Dr. Newill and his team help American soldiers survive by helping develop more accurate projectiles.

Gun/projectile dynamic simulations have been in development at the U.S. Army Research Laboratory (ARL) since the 1950s but were severely handicapped by the available computing power. As the computing power increased, the detail and complexity of the models increased, but it wasn't until the late 1980s that both the computing power and technology were available to provide detailed three-dimensional physics based models that can capture the details of projectile launch. In the late 1980s, Dr. Bruce Burns started the development of the fully three-dimensional projectile launch dynamic techniques through Dr. Don Rabern at Lawrence Livermore National Laboratory.

In the early 1990s, Dr. Steve Wilkerson brought that technology to ARL and expanded the approach to include the entire M256 gun with operating recoil system. This allowed Dr. Wilkerson to investigate attributes of the
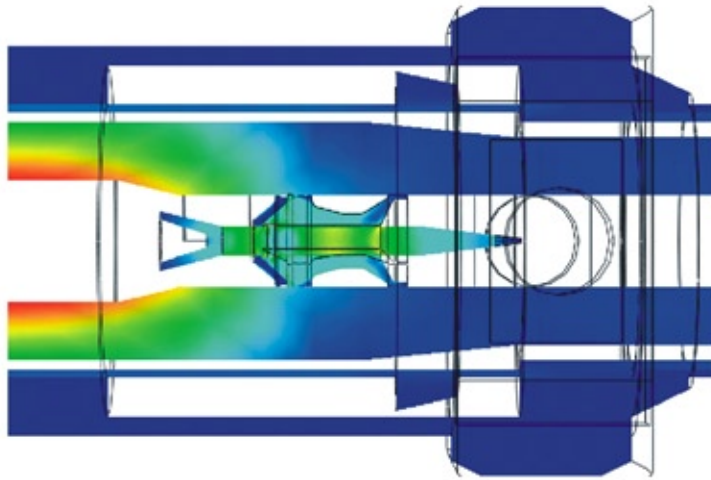
M865 near peak pressure.

gun/projectile system that contribute to variability at muzzle exit. Dr. Wilkerson also showed how different modifications could dramatically alter the dynamics of the system and the importance of gun tube centerline shape.

Dr. Newill has expanded on this technology by developing the methodology to explain and define the system accuracy performance of projectiles, which has been validated through precision jump testing. In fact, the Aerodynamics Branch has done six jump experiments over the last seven years from which Dr. Newill used a series of orthogonal muzzle X-rays to validate the predicted projectile rates at muzzle exit against the experiments. It should be noted that while the methodology and experiments were instrumental to application of these techniques, it was also simultaneous rapid expansion and application of ARL's MSRC computing power that made this technology work.

In this of type work, a successful outcome is measured in terms of incorporation of results from research into production projectiles. Results from gun/projectile dynamic simulations work have been integrated into production for various projectiles in the 120-mm family; therefore, Dr. Newill's work is certainly considered a success for the Army and the DoD.

The first projectile where the technique was used extensively was the kinetic energy projectile, the M829A2, or the A2. For the A2, Dr. Wilkerson showed that proposed modifications to the forward bourrelet would slightly improve the accuracy performance of the projectile. The modification was required to fix problems related to environmental conditioning. While the result did not show improvements in accuracy, it reassured the community that the required modifications would not affect the performance of the projectile. (These results were confirmed through ballistic testing.)

Dr. Newill showed that the diameter of the forward bourrelet could be reduced again without impact

to the accuracy performance. This result was counterintuitive to the predominate thinking in the community, but the simulation result was validated through large-scale ballistic testing. Simulation also showed (again validated through jump testing) that the M829A2 had more variability in rates at muzzle exit than the M829A1, the previous generation. As part of this work, it was not only shown that the design of the forward bourrelet was cause of the variability, but it also developed approaches to modify the forward bourrelet to reduce the variability. This work was carried into the design of forward bourrelet for the M829A3.

The M829A3 was also the first projectile to use the gun codes from the start of the program through the entire development cycle. The gun codes were used to study each attribute of the launch projectile to help determine the sensitivity to launch accuracy. At the end of the development, Bob Darcy (M829E3 Integrated Product Team Leader, responsible for the cartridge development for Project Manager – Maneuvering Ammunition Systems [PM-MAS], formally PM Tank Main Armament Systems), stated this "projectile has the best accuracy performance of any of the 120-mm KE projectiles at the beginning of production."

In addition, several other projectiles have used the gun codes and benefited from the resources available at the ARL MSRC. The XM1002, the multipurpose anti-tank (MPAT) training projectile, has used the gun codes to assess performance through the entire development cycle. When "down selecting" from different configurations of prototypes, the gun codes were used to show that a smaller projectile with a lower moment of inertia typically had high rates from balloting at muzzle exit. For the M865, the kinetic (KE) training projectile, the gun codes have been used to assess the sensitivity of the performance to bourrelet diameter and how the obturation system can affect performance, both of which were validated through ballistic testing. For the M831A1, the HEAT training projectile, simulations were used for obturation modification and to show the sensitivity of the projectiles performance to launch from worn gun tubes.

One of the other ways for Dr. Newill's team to measure success is achieving "type classification" of rounds, which shows that the Army has accepted the projectile and it is ready for full rate production. The M829A3 was type classified in February 2003, and the XM1002 is expected to be type classified by the end of 2003. Both rounds used the gun dynamics codes for their development and design, and both rounds perform very well.

Dr. Newill's work is part of an ongoing effort to cut cost and speed up the process for the DoD. Dr. Newill and his team used the HPC resources at the ARL MSRC to save time and money.

"We would not exist without MSRC resources. It'd be impossible for our group to procure the assets to do these calculations on our own," says Dr. Newill. He goes on to say, "There is no doubt we've done things faster using HPC resources, but that is the timeline being demanded by the development community. The development of the XM1002 round was completed from start to finish in 3 years, which is extremely fast for a bullet."

Prototype KE launch using NGEN propellant loading
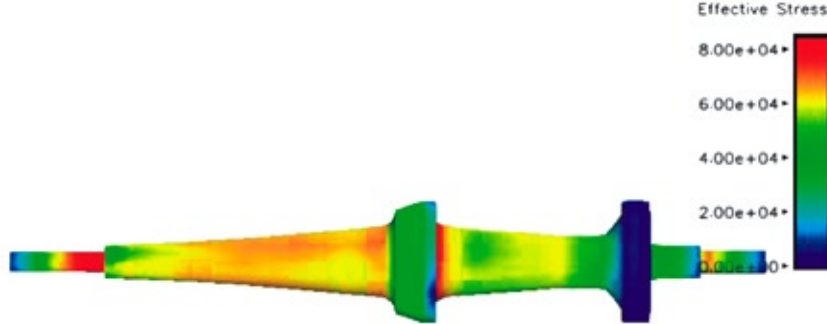
Coupled NGEN internal ballistic simulation with the gun codes.

Furthermore, Dr. Newill and his team credit the ARL MSRC and its hard-working and dedicated team of professionals for aiding in their success. "This work would not be possible without the large team of folks at the MSRC," explained Dr. Newill.

In addition to the personnel at the ARL MSRC, Dr. Newill and his team utilized the MSRC's software. Dr. Newill explains that he "used a lot of custom software, also Dyna3D, CFD [computational fluid dynamics] codes like NGEN, codes for data reduction, etc."

Dr. Newill points out that one example of the tremendous cost-cutting results that came out of working with the gun codes and the ARL MSRC resources can be seen in the development of the E3 round, which was done with two-thirds the numbers of rounds used in the previous generation development. He told us that "part of the reduction was due to the simulation work done at the ARL MSRC. With the MSRC, I was able to run over 6,000 simulations for the program. PM-MAS estimated the direct savings from the simulations was $4.2 million with this work."

To provide additional perspective on the cost savings, if just 2,000 of these projectiles had actually been built and fired, instead of just simulated using HPC resources, the cost savings would have been more than three times this amount (extension of the program, personnel, and testing costs) and it would have added several years to the program. In addition, Dr. Newill explained that another part of the impact is that "we were able to explore many concepts that could not have been accommodated within a traditional development program."

So, what does the future hold for Dr. Newill and his team? Currently, Dr. Newill and his team are working in smart munitions and coupling their gun dynamic codes with CFD codes. This allows them to investigate the effects on the structure of a projectile, such as a fin or canard, when it's subjected to supersonic flow, or what happens to the projectile structure (and embedded electronic components) when jet thrusters are fired. In the coming years, they will be working more and more with guided and smart munitions.

One example of this is Dr. Newill and Dr. Michael Nusca (ARL BWCD) work to couple Nusca's next generation interior ballistics code (NGEN) to the gun codes. NGEN can predict full three-dimensional combustion of the advanced propellants that are used in state-of-the-art projectiles. This coupled capability allows the study of asymmetric pressure effects (transverse and radial pressure waves) on launch of a projectile that result from imperfect conditions during combustion, which represent a major step in studying the effect of propellant ignition and burning on the projectile in-bore.

Dr. Newill is also working with Aerospace Engineers Dr. Paul Weinacht and Dr. Jubaraj Sahu (both of ARL BWCD) on coupled computational fluid dynamics/structural dynamic simulations that are related to guided projectiles (e.g., effects of thruster jets and defecting guidance canard on the structure of a flight body). In addition, Dr. Newill's work with Mr. Alex Zielinski (of the Army's 6.2 EM Projectile program, ARL BWCD) and Dr. John Powell (ARL TED) means that these technologies have been extended into launch of EM projectiles, through coupling an electromagnetic code (developed by Dr. Powell) to the gun codes for prediction of the survival and accuracy performance of the projectile. EM projectiles are proposed technology for the Army's Future Combat System (FCS). Other FCS technologies include use of this technology to help develop the new lightweight guns for FCS like the XM36, 120-mm smooth bore cannon (well-designed guns are paramount to achieve the system performance requirements); the multipurpose, extended range munition; and the smart cargo munition.

Thanks to the hard work of Dr. Newill and his team, along with the dedicated personnel and computing power at the ARL MSRC, projectiles will continue to increase in accuracy and precision. This means better performance in the field, which translates to survivability for the U.S. warfighter. Dr. Newill and his team continue to close in on their goal and the goal of the warfighter: one shot, one kill.

New Visualization Center Opens at APG

by Rick Angelini and Mark Bolstad

In early December, 2002 installation of the RAVE-II Immersive display system in the new ARL MSRC Scientific Visualization Center was gearing up. Of paramount interest in the early part of the installation was getting a 20-foot piece of glass lifted into the 3rd floor facility. This delicate process was complicated by high winds and an early season snow storm which temporary stranded both the crane and the flatbed trailer hauling the glass. Aside from these early weather related incidents, the installation by SGI and Fakespace was flawless and was completed on December 20, 2002. (A complete description of the RAVE-II system was included in our Fall 2002 issue.)

Pioneer usage of the reconfigurable display system began immediately and several applications were able to immediately take advantage of this new immersive technology.

Ensight Gold, from Computational Engineering International, has a flexible interface for defining a multiple pipe display environment and supports the RAVE-II in both the "wall" (opened) and "cave" (closed) environment. Ensight Gold also supports head tracking and 6 DOF (degree of freedom) input devices such as a wand, both of which are critical to supporting interaction in an immersive environment. Ensight is used extensively at the ARL MSRC as a general purpose visualization tool, and all Ensight-compatible datasets can be visualized using the RAVE-II immersive display.

Another package which was initially tested was Xmovie, an application written at the Lawrence Livermore National Laboratory. Xmovie is a multi-threaded, multi-pipe application for playing back "movies" prepared especially for large, multi-pipe display environments. Xmovie provides stereo playback across the wall including the floor projection of the RAVE display.

RAVE II display system in cave configuration.

Visual Molecular Dynamics (VMD) is Open Source software from University of Illinois at Urbana-Champaign that is used to support Computational Chemistry visualization. The CAVE variant of VMD directly supports the head tracker and wand interface used at ARL and provides a truly immersive environment for visualizing molecular structures. Early implementations have been very positive, providing a unique experience that allows the researcher to stand inside of a molecule and interact with the structure.

RAVE II display system in wall configuration.

For application development, there are several free and commercial software libraries for building RAVE applications. The two most promising are CAVElib from VRCO and a suite of tools from SGI. CAVElib has been in use for many years and abstracts the process of developing for four simultaneous views plus interaction with the wand and head tracker. SGI provides a toolkit called Performer, an API used by many for developing visual simulations. Performer is capable of multi-pipe, multi-processor application for real-time graphics. The availability of CAVElib, SGI's MultiPipe Toolkit, and the Visualization Toolkit (VTK) provides numerous options for creating a framework for multi-pipe-aware custom visualization software.

Starting in March, the second phase of the RAVE implementation will begin. In this phase, FakeSpace and SGI will integrate the existing ARL MSRC audio and video assets into a structure that will allow these input sources to be displayed on the RAVE.

ARL MSRC Builds the HPC Room at the 23rd Army Science Conference

By Brian Simmonds

The first week of December found members of the ARL MSRC Conference Support Team and other MSRC staff in Orlando, Florida, for the 23rd Army Science Conference. The conference, which was from 2-5 December, was a chance for ARL as well as the other Army supercomputing centers to show how HPC is an essential and important component of Army research.

The story starts several months prior. A request was received from Dr. John A. Parmentola, Special Assistant to Deputy Assistant Secretary for Research and Technology, for ARL to put together an Army Supercomputing display and demonstration area for the conference. Management and team members were already in a full-steam-ahead planning mode for the Supercomputing 2002 booth. It was decided that the equipment and many of the demonstrations could be used at both shows. Immediate planning of the booth space and footprint layout began. After several locations failed to be suitable, it was decided that the displays would be in the hotel atrium. With assistance and support from the Army Material Command (AMC) Exhibits group, who had been tasked with the AMC technologies displays, the configuration and design was settled. The next tasks were to get in touch with the other Army Supercomputing groups and centers and plan the demonstrations, speakers, and briefings.

Through generous equipment loans, manufacturer support, rentals, and the efforts of the MSRC Conference Support Team, the booth took shape. Many of the pieces arrived on site only 24 hours before the booth was to be active. Administrators as well as technical support people from all of the centers worked well into the night to ready the demonstration hardware and software to support the scientific application demos. The high-end devices and computers were all ready for the 6:00 PM opening reception.

Many high-ranking Department of the Army personnel attended, including General John M. Keane, Vice Chief of Staff, U.S. Army; Claude M. Bolton, Jr. Assistant Secretary of the Army for Acquisition, Logistics and Technology; General Paul J. Kern, Commanding General, U.S. Army Materiel Command; as well as our own Dr. Robert Whalin and Dr. N. Radhakrishnan.

The booth contained several high-end display technologies to display the computer-generated graphics. A 3-meter Elumens Vision Dome was one of the more unconventional devices on hand. The Vision Dome is a hemispherical projection screen with a projector mounted in the front to give a 160-degree immersive environment that allows the viewer's peripheral vision to be filled. The second display was a rear projection Mechdyne Portable. This billboard-sized display was 3D capable (with the special glasses) and was connected to an SGI Onyx 3800 IR3 computer. The third display device was a Fakespace Immersadesk R3. This device was also 3D capable and was used to give informal talks as well as formal presentations.

In keeping with the theme of the conference, "Transformational Science and Technology for the Army … a race for speed and precision," the booth had several other attractive elements. The Lightstage was a real draw. This lighted, ball-shaped device attracted attendees as well as other exhibiters (see sidebar). An interactive touch-screen plasma display gave visitors on-demand information about the Army Supercomputing Centers and many of their projects. A history of Army Supercomputing display was also there to show the evolution of the supercomputing hardware.

The real booth attractions were the talks and demonstrations. Numerous scientists and researchers from each of the Army Centers presented their work and associated animations and graphics. Large groups formed to listen and see the science being demonstrated as well as interact with peers in their fields.
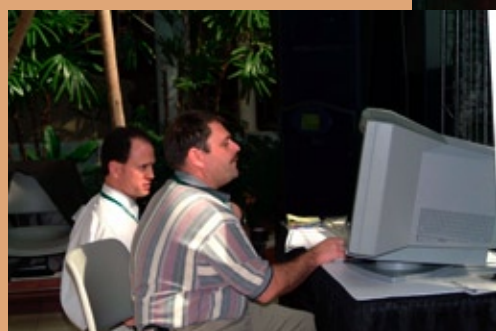
Electromagnetic Code Consortium at the ARL MSRC

By Dr. Charles Macon

The Electromagnetic Code Consortium (EMCC) was chartered under a joint agreement between the DoD services and NASA and is comprised of members from the Army, Navy, Air Force, and NASA. The role of the EMCC is to develop and transition basic Computational Electromagnetic (CEM) research activities. The EMCC supports the applications users, centralizes the dissemination of CEM codes, develops basic CEM technology, baseline codes, validation tools and data, benchmark cases, and establishes validation procedures for CEM technologies. The Government Executive Committee (GEC) is the governing body of the EMCC.

As part of his responsibilities as the PET CEA On-site at ARL, Dr. Charles Macon (High Performance Technologies, Inc.) supports the efforts of the EMCC. He has collaborated with the EMCC GEC to install the following serial CEM codes on HPC platforms at the ARL MSRC: AIM version 1.12, CARLOS version 2.0, PARANA version 2, and RAM2D version 3.2.

AIM is a three-dimensional (3D) method of moments (MoM) code for calculating far-field scattering from various types of surfaces (e.g., PEC, IBC, R-card) and dielectric regions. CARLOS is a 3D MoM code used for calculating far-field scattering from surfaces and dielectric regions. PARANA is a hybrid finite element code for the analysis of phased array antennas, periodic structures, waveguide devices, and for calculating far- and near-field scattering from surfaces and dielectric regions. RAM2D is a two-dimensional MoM code for calculating far- and near-field scattering from surfaces and dielectric regions. AIM, CARLOS, PARANA, and RAM2D are currently installed on the SGI Origin 2000 and 3800 machines. PARANA is installed on the IBM SP3.

These codes are export controlled. Export-controlled information or material is any information or material that cannot be released to foreign nationals or representatives of a foreign entity without first obtaining approval or license from the Department of State for items controlled by the International Traffic in Arms Regulations (ITAR). Pursuant to this classification, warnings and restrictions apply. In addition, violations of these export laws are subject to severe criminal penalties. For more information about export-controlled information or material, please contact the ARL MSRC help desk at 1-800-275-1552 or via email at msrchelp@arl.army.mil.

Due to the export controls on the EMCC codes, the following procedure was established in collaboration with the EMCC Chair and the ARL MSRC. Access to these
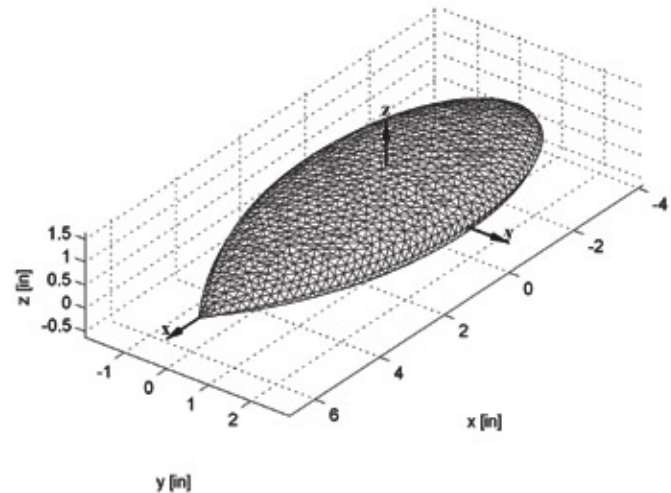

Figure depicts the discretized surface of the 9.936-inch NASA almond test body.

codes at the ARL MSRC is to be granted only to users who have signed the EMCC software license (available from EMCC's Web site) and had the license approved by the EMCC Chair. Moreover, software license forms submitted to the EMCC Chair by non-government employees must be accompanied by a copy of a DD Form 2345 (Militarily Critical Technical Data Agreement) with a valid certification number in block 7 of that form.

Users who contact the ARL MSRC to request access to the codes are referred to the EMCC Chair and access is granted upon notification from the EMCC Chair to Dr. Macon and the ARL MSRC help desk. Upon the conclusion of the tenure of an EMCC chair, the name and contact information of the succeeding chair is provided to Dr. Macon.

The procedure outlined above was reviewed and approved by Ms. Denice Brown, Deputy Director and Information Assurance Security Officer, ARL, MSRC, in August 2002. For further information on the use of these codes, please contact Dr. Charles Macon at 410-278-9282 or via e-mail at cmacon@arl.army.mil.

Buddy, Can You Spare a Patch?
By CIMP Staff

Our previous CIMP column was a plea for our end-user community to consult local IT support staff before installing or upgrading software on their systems. With this edition, we turn our attention to our harried support staff.

In the early hours of January 25, 2003, the computer security world became painfully aware of a new Microsoft SQL worm that perpetrated a denial-of-service attack at sites with infected hosts. Microsoft SQL Server is a relational database management and analysis package that allows sharing of database information over the Internet. With the introduction of Microsoft SQL Server 2000, Microsoft added support for multiple instances of SQL Server on a single host and implemented a rendezvous protocol for locating specific SQL servers on that host. It was the rendezvous protocol that was the target of the worm.

Slammer (a.k.a. Sapphire or SQLSlammer) took everyone by surprise. Propagation reports showed the number of infected hosts doubled every 10 seconds, and tens of thousands of hosts were infected. For the first time, significant collateral damage was observed in seemingly unrelated services, such as the Bank of America automated teller network, which was unavailable for nearly two days, and the SouthWest Airlines reservation system, which was unable to process transactions for several hours. Slammer also exacted a toll on DoD. Fortunately the damage within DoD was relatively minor and, other than some substantial traffic loading for a few hours, very limited in extent.

For the hosts that were hit, this worm was largely benign -- and on that score we were very lucky. The worm made no attempt to install itself in a manner that re-infected the system upon reboot, and no permanent files or registry settings were written or altered. The only action necessary to stop propagation was to filter the IP port and block the infected host until it could be patched. On any infected host, the worm could be removed by simply rebooting the system.

The unfortunate part of this story is that the underlying vulnerability was publicized last summer, and DoD issued an IAVA Bulletin addressing this weakness in September.

It was a "Bulletin" not an "Alert," but there were specific instructions detailing how to mitigate the problem -- sounds like "shame on our system administrators."

Yet, the story is seldom as clear-cut as it seems. Even if every one of our administrators had carefully patched every affected system, all was not well because Microsoft released subsequent updates that undid the patches in some cases. Given these circumstances, it was inevitable that some systems would succumb to the worm.

The tip for this quarter is for system administrators to be vigilant in assuring that all necessary patches and updates are installed as soon as available, and to ask for explanations from peers and other IT staff when a machine is found in an unexpected state. Hasty reaction may undo steps others have taken to protect the infrastructure.

For details about Information Assurance across DOD and specifically the most recent alerts and bulletins, please visit

ftp://www.cert.mil/pub/bulletins/iava/iava_index.htm

The Army site for computer emergency information is

https://www.acert.1stiocmd.army.mil/

The Air Force link for this information is

https://afcertmil.lackland.af.mil/

The Navy link for Information Assurance is

https://infosec.navy.mil/

ARL MSRC Help Desk Gets a Boost From New Remedy

By Dr. Robert Cromp

The ARL MSRC Help Desk uses a software package known as Remedy to record and track active help requests. Recently, this Remedy software has undergone a major new release, providing us an opportunity to improve our Help Desk services by taking advantage of the new features. Most of the changes will be invisible to the user community but will enable us to develop better tools for detecting trends in problem areas due to a cleaner integration of Remedy with the underlying Oracle database system.

One very prominent change will be that users will be able to submit, track, and update their requests for help through a Web interface (along with the typical email and phone submissions currently employed). Currently, Remedy is used only by the front-line Help Desk personnel. The new version of Remedy will be extended throughout several teams of the ARL MSRC support staff to include the Help Desk, System Administration, Applications Support, and Scientific Visualization teams.

Figure 1 Support request form showing contextual menu.

Figure 1 shows a form from the Web site for a user to report a problem or request help. The user categorizes the type of request, and a context-dependent menu of services for the chosen category is automatically generated. After selecting a specific service for the given category, the user provides additional information relevant to the request. Upon authenticating to the system, the help request is submitted to Remedy where it is logged as a new "ticket" and directly channeled to the appropriate Customer Support team for action and resolution. In return, Remedy provides a confirmation notice to the user summarizing the ticket. Remedy also supplies information on how the user can

interact via the Web to track the ticket's status and provides additional data, if necessary. Within a short amount of time, a member of the Customer Support team needs to formally accept the ticket through a Remedy interface, indicating that the help request has been scoped correctly; occasionally the ticket may need to be recategorized and passed to another group on the support staff.

Accepted tickets are actively worked by individuals until a solution is found. For particularly complex problems, several iterations may occur where the user is asked to supply additional information in order for the support staff to eliminate possible problem causes until a potential solution is found. The solution is provided to the user, and the user is asked to certify that the problem is solved. If the user agrees, the ticket is closed; otherwise, the ticket is updated to reflect why the proposed solution is deficient and the support staff delves further into the problem until a solution satisfying the user's request is found.

Users will also be asked to rate the quality of service with respect to suitability of the solution, time required to solve the request, and overall interaction with the ARL MSRC support staff.

Over time, numerous statistics will result, including the expected amount of time necessary for resolving each category and service of problem. Support staff will use this information to establish goals for solving individual tickets. Tickets resisting solution can be formally escalated so that ARL MSRC management can be notified automatically and additional resources brought to bear. Additionally, as the corpus of knowledge on problem types and their solutions is accrued, certain solution patterns will become evident, allowing standard operating procedures (SOPs) to be developed for commonly occurring help requests. These SOPs can be formalized and provided automatically to users when they submit queries that match against them.

Integration of the new Remedy into the Help Desk should be complete and available to the general ARL MSRC user community in mid May.

Grid Engine Script Generating Tool Now Available for Users

By Dr. Robert Cromp and Jeffrey Robinson

Most high performance computing centers use a batch queuing system to facilitate job throughput by matching computer resources against job requirements. Users typically communicate their job constraints to the queuing system by writing a job submission script. This scripting task can be frustrating to some users because errors can keep the script from submitting the job properly, or cause the queuing system to handle the job differently than how the user intended.

At the ARL MSRC, we have recently developed and released the Grid Engine Script Generating Tool (GEST) to help users produce batch scripts for ARL's most-utilized COTS software packages. Users supply information through GEST's graphical user interface (GUI), permitting them to concentrate on their functional area knowledge of the application software instead of the low-level scripting details for defining and submitting jobs. GEST imposes a framework across all applications, dynamically configuring the GUI for application-specific inputs based on information entered by the user. Context-sensitive help messages automatically appear as the user selects each input field, and HTML-based documentation can also be viewed. GEST has the ability to save preferences that can be reloaded and modified at a later time, a worthwhile feature since users tend to use a given software package multiple times with similar settings. Scripts subsequently generated can be submitted directly, or saved for further customization by the user.

GEST is designed so that new applications can be easily added. A customization file delineates the possible inputs, associated GEST actions (such as default values, help messages, structure of application invocation command line), and GEST GUI layout for each supported application. Although written with respect to Grid Engine, GEST can be configured to work with other batch systems such as Load Leveler, PBS, and LSF.

GEST also captures statistics that allow the ARL MSRC to better assess how the tool is being used and the amount of time consumed by each user with its various features. The understanding garnered through analyzing this data should be beneficial in devising improvements and enhancements to future releases of this software.

Screen shot of the GEST interface.

GEST allows users to avoid the typical mistakes that can occur when they write their own scripts. It significantly reduces the amount of time that users spend writing and debugging scripts. By using GEST, users should be able to minimize and, in most cases, eliminate incorrect runs from improperly constructed submission scripts, resulting in more effective use of the overall computing resources.

Access GEST documentation
at this URL:

http://www.arl.hpc.mil/docs/gest/

Team Efforts Create Conference Success
By Michelle Morgan-Brown

This fall, the ARL MSRC attended both the Supercomputing 2002 (SC2002) and Army Science conferences. SC2002 was in Baltimore, MD, and the Army Science Conference was in Orlando, FL. Due to a solid team effort, both conferences were a big success.

For SC2002, the ARL MSRC sponsored the HPCMP booth, which featured Plasma displays, a portable Immersadesk, and the 3 meter Elumens VisionDome. Also displayed at SC2002 were the Land Warrior, a state-of-the-art system for the warfighter and part of the Army's Future Combat System, and one of the Army's newest vehicles, the Family of Medium Tactical Vehicles (FMTV) truck.

Of course, all of these neat displays, demos, and new technologies don't run by themselves. The ARL MSRC is fortunate to have some wonderful people who made all

of this possible through their hard work, long hours, time away from home, and dedication to duty. A big thanks goes out to our conference support team for making sure everything ran smoothly at SC2002 and the Army Science Conference.

Special thanks go to Tom Kile and Judy Bouchelle-Keithley. Tom was the Network Engineer responsible for the design and implementation of wide area networks between the Baltimore Convention Center, where SC2002 took place, and all of our external centers. Judy, our Outreach Lead, also coordinated technical content and support between the HPCMO, the four MSRCs, and many Distributed Centers.

A lot of credit goes to the rest of our team, too:

- Tom Brezee, logistical and technical support coordination
- Mark Bolstad, lead developer for scientific visualization and technical content for Army Science Conference
- Dr. Robert Cromp, lead for technical production and content for Army Science Conference
- Randy Dalnekoff, technical and logistical support for vendors, SC2002 committee, and suppliers
- Eia Dobbins, administrative support, supplier contracts, and coordination of all attendees, local accommodations, and registration
- Bob Horner, hardware installation and PC/workstation setup and configuration. Bob also drove the equipment truck to and from ARL to SC2002 as well as to Orlando and back. Thanks, Bob!
- Mark Motsko, hardware installation and integration and LAN support
- Susan Neczyporuk, integration of Adelphi visualization products and displays
- Jim Nelson, editing of video productions and support of audio/visual equipment and displays
- Carl Rossmark, system administration and setup of visualization systems
- Randy Schauer, Web site and Web page development and administration
- Brian Simmonds, technical, multimedia, outreach, and support
- John Vines, audio/visual design and implementation

Upcoming Events

Conferences and Symposiums

9 to 13 June 2003 (Conference): DoD HPCMP Users Group Conference 2003
Location: Doubletree Hotel, Bellevue, Washington. Hosted by HPCMP.
For more information: http://www.hpcmo.hpc.mil/Htdocs/UGC/UGC03.

22 to 23 July 2003 (Symposium): On the Use of Commodity Clusters for Large-Scale Scientific Applications
Location: Holiday Inn, Tysons Corner, Virginia. Hosted by ARL MSRC, Raytheon, and OSC.
For more information: http://www.arl.hpc.mil/Clusters2003.

8 to 11 September 2003 (Conference): 6th Annual SMART Conference and Exhibit
Location: Hyatt Regency Hotel, Dearborn, Michigan.
For more information: http://www.amso.army.mil

PET Events at ARL

PET events at ARL MSRC and other centers can be accessed through the Online Knowledge Center at

https://okc.erdc.hpc.mil

The MSRC Help Desk
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Connecting Users to the ARL MSRC

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Major Shared Resource Center (AMSRL-CI-H)

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